Integral representation of von Neumann entropy

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Abstract

By using an integral formula, we easily calculated the von Neumann entropy of any quantum state.

1 Introduction

The expression for von Neumann entropy[1]-[2] is

$$S(\rho) = -Tr\rho \ln \rho. \tag{1}$$

where ρ is the density matrix of any quantum state. Now, we introduce an integral formula

$$\frac{1}{\pi}\int_0^\infty \ln x \ln(1+\frac{a^2}{x^2})dx = a\ln a - a, \quad a>0. \tag{2}$$

Since any density matrix ρ is semi positive definite, without loss of generality, we get

$$-\rho\ln\rho = -\rho - \frac{1}{\pi}\int_0^\infty \ln x \ln(\mathbf{1}+\frac{\rho^2}{x^2})dx. \tag{3}$$

Tracing both sides of Eq. (3), we have

$$\begin{aligned} S(\rho) &= -Tr\rho\ln\rho \\ &= -Tr\rho - \frac{1}{\pi}\int_0^\infty \ln x Tr\ln(\mathbf{1}+\frac{\rho^2}{x^2})dx. \end{aligned} \tag{4}$$

According to the formula $Tr\ln\mathbf{A} = \ln\det\mathbf{A}$, Eq. (4) can be changed as

$$S(\rho) = -Tr\rho - \frac{1}{\pi}\int_0^\infty \ln x \ln\det(\mathbf{1}+\frac{\rho^2}{x^2})dx, \tag{5}$$

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which is exactly the integral representation of von Neumann entropy $S(\rho)$, where $\det(\mathbf{1}+\frac{\rho^2}{x^2})$ is a Fredholm determinant in fact. For a Fredholm determinant of n multiplied by n matrix, there is the following expansion formula:

$$\det(\mathbf{I}+t\mathbf{A}) = \left\{ \begin{array}{c} \mathbf{I}+tTr\mathbf{A}+t^2\det\mathbf{A}, \quad n=2 \\ \mathbf{I}+tTr\mathbf{A}+\frac{t^2}{2!}[(Tr\mathbf{A})^2-Tr\mathbf{A}^2]+t^3\det\mathbf{A}, \ \ n=3 \\ \mathbf{I}+tTr\mathbf{A}+\frac{t^2}{2!}[(Tr\mathbf{A})^2-Tr\mathbf{A}^2] \\ +\frac{t^3}{3!}[(Tr\mathbf{A})^3-3(Tr\mathbf{A})(Tr\mathbf{A}^2)+2(Tr\mathbf{A}^3)]+t^4\det\mathbf{A}, \ \ n=4 \\ \cdots . \end{array} \right\} \tag{6}$$

Then, for $n=2$,

$$\begin{aligned} \det(\mathbf{1}+\frac{\rho^2}{x^2}) &= 1+\frac{Tr\rho^2}{x^2}+\frac{\det\rho^2}{x^4} \\ &= 1+\frac{Tr\rho^2}{x^2}+\left(\frac{\det\rho}{x^2}\right)^2 . \end{aligned} \tag{7}$$

For $n=3$,

$$\begin{aligned} \det(\mathbf{1}+\frac{\rho^2}{x^2}) &= 1+\frac{Tr\rho^2}{x^2}+\frac{[(Tr\rho^2)^2-Tr\rho^4]}{2!x^4}+\frac{\det\rho^2}{x^6} \\ &= 1+\frac{Tr\rho^2}{x^2}+\frac{[(Tr\rho^2)^2-Tr\rho^4]}{x^4}+\left(\frac{\det\rho}{x^3}\right)^2 . \end{aligned} \tag{8}$$

For $n=4$,

$$\begin{aligned} & \det(\mathbf{1}+\frac{\rho^2}{x^2}) \\ = \ & 1+\frac{Tr\rho^2}{x^2}+\frac{[(Tr\rho^2)^2-Tr\rho^4]}{2!x^4} \\ & +\frac{[(Tr\rho^2)^3-3(Tr\rho^2)(Tr\rho^4)+2(Tr\rho^6)]}{3!x^6}+\left(\frac{\det\rho}{x^4}\right)^2 . \end{aligned} \tag{9}$$

It is already known that any pure state satisfies $\rho^2=\rho$, so

$$Tr\rho = Tr\rho^2 = Tr\rho^n = 1. \tag{10}$$

According to Eq. (5), we show that for n by n density matrix ρ for a pure state,

$$\begin{aligned} S(\rho) &= -Tr\rho-\frac{1}{\pi}\int_0^\infty \ln x\ln\det(\mathbf{1}+\frac{\rho^2}{x^2})dx \\ &= -1-\frac{1}{\pi}\int_0^\infty \ln x\ln[1+\frac{1}{x^2}+\left(\frac{\det\rho}{x^n}\right)^2]dx. \end{aligned} \tag{11}$$

The result of Eq. (11) is very concise and beautiful.

For any pure state, because

$$\det\rho^2 = (\det\rho)^2 = \det\rho, \tag{12}$$

so,

$$\det \rho = 0, 1. \tag{13}$$

As we all know, $\det \rho$ can only be 0 for any pure state, thus its von Neumann entropy $S(\rho) = 0$.

2 Eigenspectrum expression of $S(\rho)$

A similar transformation $\mathbf{P}$ can always be found to diagonize the density matrix ρ. Let the diagonalized matrix be $\mathbf{D}$, then

$$\mathbf{P}^{-1}\rho\mathbf{P} = \mathbf{D} = diag(\lambda_1, \lambda_2, \ldots, \lambda_n), \tag{14}$$

where λ_i is the eigenvalue of ρ. We have

$$\begin{aligned}
\det(\mathbf{1} + \frac{\rho^2}{x^2}) &= \det[\mathbf{P}^{-1}(\mathbf{1} + \frac{\rho^2}{x^2})\mathbf{P}] \\
&= \det(\mathbf{1} + \frac{\mathbf{D}^2}{x^2}) \\
&= \prod_{k=1}^{n}(1 + \frac{\lambda_k^2}{x^2}).
\end{aligned} \tag{15}$$

then

$$\begin{aligned}
S(\rho) &= -Tr\rho - \frac{1}{\pi}\int_0^\infty \ln x \ln\det(\mathbf{1} + \frac{\rho^2}{x^2})dx \\
&= -1 - \frac{1}{\pi}\int_0^\infty \ln x \ln\prod_{k=1}^{n}(1 + \frac{\lambda_k^2}{x^2})dx \\
&= -1 - \frac{1}{\pi}\sum_{k=1}^{n}\int_0^\infty \ln x \ln(1 + \frac{\lambda_k^2}{x^2})dx \\
&= -1 - \sum_{k=1}^{n}(\lambda_k \ln\lambda_k - \lambda_k) \\
&= -\sum_{k=1}^{n}\lambda_k \ln\lambda_k,
\end{aligned} \tag{16}$$

which is consistent with the traditional expression of $S(\rho)$.

3 Series expansion of $S(\rho)$

Usually, the computation of solving the eigenvalue of density matrix ρ is very large, so we try to find a simpler way to calculate von Neumann entropy $S(\rho)$ to reduce the computation. Based on the form given by Eq. (4), we speculate

whether it is possible to rewrite $S(\rho)$ into some series form. Firstly, we should consider

$$\ln(\mathbf{1} + \frac{\rho^2}{x^2}) = -\sum_{k=1}^{\infty} \frac{(-\frac{\rho^2}{x^2})^k}{k}, \tag{17}$$

then

$$Tr \ln(\mathbf{1} + \frac{\rho^2}{x^2}) = -\sum_{k=1}^{\infty} \frac{(-1)^k Tr \rho^{2k}}{k x^{2k}}. \tag{18}$$

However, unfortunately, by substituting Eq. (18) into Eq. (4), we found that the integration is divergent. To make up for this deficiency, we try to write the integral in Eq. (2) form in piecewise form and use the substitution method to perform some deformation treatment on the integral, which means

$$\begin{aligned} & \int_0^{\infty} \ln x \ln(1 + \frac{a^2}{x^2}) dx \\ = & \int_0^1 \ln x \ln(1 + \frac{a^2}{x^2}) dx + \int_1^{\infty} \ln x \ln(1 + \frac{a^2}{x^2}) dx \\ = & \int_0^1 \ln x \ln(1 + \frac{a^2}{x^2}) dx - \int_0^1 \frac{\ln x \ln(1 + a^2 x^2)}{x^2} dx. \end{aligned} \tag{19}$$

However, the first integral of Eq. (19) after written as the series form is still divergent, so we have to continue to transform it into the following form

$$\begin{aligned} & \int_0^1 \ln x \ln(1 + \frac{a^2}{x^2}) dx \\ = & \int_0^1 \ln x \ln(x^2 + a^2) dx - 4 \\ = & \int_0^1 \ln x \ln(1 + \frac{x^2}{a^2}) dx + 2 \ln a - 4. \end{aligned} \tag{20}$$

Thus,

$$\begin{aligned}
&\int_0^\infty \ln x \ln(1+\frac{a^2}{x^2})dx \qquad (21)\\
=\;& \int_0^1 \ln x \ln(1+\frac{x^2}{a^2})dx - \int_0^1 \frac{\ln x \ln(1+a^2x^2)}{x^2}dx + 2\ln a - 4\\
=\;& -\int_0^1 \ln x \sum_{k=1}^{\infty}\frac{(-\frac{x^2}{a^2})^k}{k}dx + \int_0^1 \frac{\ln x}{x^2}\sum_{k=1}^{\infty}\frac{(-a^2x^2)^k}{k}dx + 2\ln a - 4\\
=\;& \sum_{k=1}^{\infty}\frac{(-a^2)^k}{k}\int_0^1 \ln x\cdot x^{2k-2}dx - \sum_{k=1}^{\infty}\frac{(-a^{-2})^k}{k}\int_0^1 \ln x\cdot x^{2k}dx + 2\ln a - 4\\
=\;& \sum_{k=1}^{\infty}\frac{(-a^2)^k}{k(2k-1)^2} - \sum_{k=1}^{\infty}\frac{(-a^{-2})^k}{k(2k+1)^2} + 2\ln a - 4\\
=\;& \sum_{k=1}^{\infty}\frac{(-1)^k}{k}[\frac{a^{2k}}{(2k-1)^2} - \frac{a^{-2k}}{(2k+1)^2}] + 2\ln a - 4.
\end{aligned}$$

We notice that $a^{-2k} = \sum_{l=0}^{\infty}(1-a^{2k})^l$ for $a<1$ and that series $\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\frac{a^{2k}}{(2k-1)^2}$ and $\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\frac{a^{-2k}}{(2k+1)^2}$ are all convergent for $a<1$, so Eq. (21) can be changed into the form as follows

$$\begin{aligned}
&\int_0^\infty \ln x \ln(1+\frac{a^2}{x^2})dx \qquad (22)\\
=\;& \sum_{k=1}^{\infty}\frac{(-1)^k}{k}[\frac{a^{2k}}{(2k-1)^2} - \frac{1}{(2k+1)^2}\sum_{l=0}^{\infty}(1-a^{2k})^l] + 2\ln a - 4.
\end{aligned}$$

Now, let a be ρ, then

$$\begin{aligned}
S(\rho) &= -1 - \frac{1}{\pi}\int_0^\infty \ln x Tr\ln(\mathbf{1}+\frac{\rho^2}{x^2})dx \qquad (23)\\
&= \frac{1}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k}{k}[\frac{1}{(2k+1)^2}\sum_{l=0}^{\infty}Tr(\mathbf{1}-\rho^{2k})^l - \frac{Tr\rho^{2k}}{(2k-1)^2}]\\
&\quad -\frac{2\ln\det\rho}{\pi} + \frac{4Tr\mathbf{1}}{\pi} - 1.
\end{aligned}$$

In this way, we simplify the calculation of von Neumann entropy $S(\rho)$ to the problem of solving the series of $Tr\rho^{2k}$ and $Tr(1-\rho^{2k})^l$, which gives us the possibility to calculate von Neumann entropy $S(\rho)$ by using numerical methods.

4 Discussion

In fact, for the problem of integral divergence caused by the series expansion of $\ln(1+\frac{a^2}{x^2})$ in equation (2), we can also use Borel resummation method to solve it. Let

$$S = \ln(1+x) = -\sum_{k=0}^{\infty}\frac{(-x)^{k+1}}{k+1} = \sum_{k=1}^{\infty} a_k, \tag{24}$$

then $a_k = \frac{-(-x)^{k+1}}{k+1}$. By using

$$\begin{aligned} S &= \int_0^\infty e^{-t}\sum_{k=0}^{\infty}\frac{a_k t^k}{k!}dt \\ &= -\int_0^\infty \frac{e^{-t}}{t}\sum_{k=0}^{\infty}\frac{(-xt)^{k+1}}{(k+1)!}dt \\ &= -\int_0^\infty \frac{e^{-t}}{t}(e^{-xt}-1)dt \\ &= \ln(1+x) \end{aligned} \tag{25}$$

and applying this method to Eq. (2), we have

$$\begin{aligned} & \frac{1}{\pi}\int_0^\infty \ln x \ln(1+\frac{a^2}{x^2})dx \\ = & -\frac{1}{\pi}\int_0^\infty \ln x \sum_{k=0}^{\infty}\frac{(-\frac{a^2 t}{x^2})^{k+1}}{(k+1)!}dx \\ = & -\frac{1}{\pi}\int_0^\infty \ln x \int_0^\infty \frac{e^{-t}}{t}\sum_{k=0}^{\infty}\frac{(-\frac{a^2 t}{x^2})^{k+1}}{(k+1)!}dtdx \\ = & -\frac{1}{\pi}\int_0^\infty \ln x \int_0^\infty \frac{e^{-t}}{t}(e^{-\frac{a^2 t}{x^2}}-1)dtdx \\ = & -\frac{1}{\pi}\int_0^\infty \frac{e^{-t}}{t}\int_0^\infty \ln x(e^{-\frac{a^2 t}{x^2}}-1)dxdt \\ = & -\frac{1}{\pi}\int_0^\infty \frac{e^{-t}}{t}\int_0^\infty \ln x(e^{-\frac{a^2 t}{x^2}}-1)dxdt. \end{aligned} \tag{26}$$

However, this solution is not conducive to solving the problem of von Neumann entropy, but rather brings considerable complexity to the problem.

Conflict of interest statement

The author does not have any possible conflicts of interest.

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